REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
17-04-2015	Final Report	1-Feb-2014 - 31-Jan-2015

4. TITLE AND SUBTITLE

Final Report: Acquisition of a High Performance Computer Cluster for Materials Research and Education

5a. CONTRACT NUMBER
W911NF-14-1-0051

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
106012

6. AUTHORS
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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)

U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
64770-EL-REP.3

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES

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14. ABSTRACT

This proposal requests funding for acquisition of a High Performance Computer (HPC) cluster to expand and strengthen the computational facility of W. M. Keck Computational Materials Theory Center (CMTC) at California State University Northridge (CSUN). The proposed HPC cluster tremendously enhanced the computational capability of CMTC and allowed the researchers to tackle challenging materials problems. The HPC cluster has been and will be used to perform first-principles simulations to predict charge carrier mobilities, exciton diffusion and interfacial charge separation in all-organic and hybrid organic-inorganic solar cells. The outcome of the project

15. SUBJECT TERMS

Computer cluster; modeling and simulations of materials

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Gang Lu
UU	UU	UU	UU		19b. TELEPHONE NUMBER 818-677-2021

Report Title

Final Report: Acquisition of a High Performance Computer Cluster for Materials Research and Education

ABSTRACT

This proposal requests funding for acquisition of a High Performance Computer (HPC) cluster to expand and strengthen the computational facility of W. M. Keck Computational Materials Theory Center (CMTC) at California State University Northridge (CSUN). The proposed HPC cluster tremendously enhanced the computational capability of CMTC and allowed the researchers to tackle challenging materials problems. The HPC cluster has been and will be used to perform first-principles simulations to predict charge carrier mobilities, exciton diffusion and interfacial charge separation in all-organic and hybrid organic-inorganic solar cells. The outcome of the project is the development of a computational capability that can potentially shift the paradigm of materials design based on time-consuming trial-and-error experiments and significantly reduce the time and labour required for materials development. The proposed cluster will also play an important role for education and training of STEM students at CSUN. Not only can the students involved in the DoD projects use the cluster, but the students taking the computational materials courses can also access the cluster for their coursework. In addition, the local high school teachers and students attending the summer camps on Computational Materials Research at CSUN will have the opportunity to use the cluster as well.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
07/28/2014	1.00	Guangfen Wu, Zi Li, Xu Zhang, Gang Lu. Charge Separation and Exciton Dynamics at Polymer/ZnO Interface from First-Principles Simulations, The Journal of Physical Chemistry Letters, (07 2014): 0. doi: 10.1021/jz500980q
07/29/2014	2.00	P. V. Ong, Nicholas Kioussis, P. Khalili Amiri, J. G Alzate, K. L. Wang, Gregory P. Carman, Jun Hu, Ruqian Wu. Electric field control and effect of Pd capping on magnetocrystalline anisotropy in FePd thin films: A first-principles study, Physical Review B, (3 2014): 0. doi: 10.1103/PhysRevB.89.094422
TOTAL:	**2**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received		Paper
TOTAL:		

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Post Doctorates

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Faculty Supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment.

Technology Transfer

Award Information

Award Number	W911NF-14-1-0051
Title of Research	Acquisition of a High Performance Computer Cluster for Materials Research and Education
Principal Investigator	Gang Lu
Organization	The University Corporation (California State University Northridge)

Technical Section

Technical Objectives

This proposal requests funding for acquisition of a High Performance Computer (HPC) cluster to expand and strengthen the computational facility of W. M. Keck Computational Materials Theory Center (CMTC) at California State University Northridge (CSUN). The proposed HPC cluster will tremendously enhance the computational capability of CMTC and allow the researchers to tackle challenging materials problems that are presently beyond the reach. The HPC cluster will be used to perform first-principles simulations to predict charge carrier mobilities, exciton diffusion and interfacial charge separation in all-organic and hybrid organic-inorganic solar cells. The first-principles simulations validated through experiments could accelerate the discovery of novel organic semiconductors for applications in photovoltaics, light-emitting diodes, flexible field-effect transistors, lighting, and displays. The proposed research involves advancement of first-principles simulation methodologies, development of user-friendly software, validation of the software through experiments, gaining fundamental understanding of underlying processes, translation of the understanding to materials design rules, and providing theoretical guidance and computational screening for rational design of materials. The outcome of the project is the development of a computational capability that can potentially shift the paradigm of materials design based on time-consuming trial-and-error experiments and significantly reduce the time and labour required for materials development.

The proposed cluster will also play an important role for education and training of STEM students at CSUN. Not only can the students involved in the DoD projects use the cluster, but the students taking the computational materials courses can also access the cluster for their coursework. In addition, the local high school teachers and students attending the summer camps on Computational Materials Research at CSUN will have the opportunity to use the cluster as well.

Technical Approach

The PI has developed a first-principles method that can predict charge carrier mobility in organic semiconductors as a function of chemical structures, presence of defects, temperature, electric field, and carrier concentration entirely from first principles; i.e., there is no empirical input or adjustable parameter in the simulations. More specifically, this approach is based on the time-domain *ab initio* non-adiabatic molecular dynamics for simulating phonon-assisted electron transitions. The electronic energy levels and their transition rates are determined from the density functional theory (DFT), taking into account of both inter-molecule and intra-molecule contributions and treating dynamic and static disorder at an equal footing. This multiscale framework incorporates quantum mechanical determination of electron transition rates, mesoscale master equations for carrier mobility and continuum models for current-voltage characteristics tailored for experimental measurements. For interfacial exciton dissociation, we have

developed a first-principle approach based on the time-dependent density functional theory (TDDFT) to describe exciton states, including energy levels and many-body wave functions. The non-adiabatic *ab initio* molecular dynamics (MD) is used to determine the phonon-assisted transition rates between localized exciton states. In conjunction with the Monte Carlo and surface-hopping methods, this approach can simulate exciton dynamics in organic semiconductors at different temperatures.

Progress:

1. Charge Separation and Exciton Dynamics at Polymer/ZnO Interface from First-Principles Simulations (Wu et al., J. Phys. Chem. Lett. 5, 2649, 2014)

Charge separation and exciton dynamics play a crucial role in determining the performance of excitonic photovoltaics. Using time-dependent density functional theory with a range-separated exchange-correlation functional as well as non-adiabatic ab initio molecular dynamics, we have studied the formation and dynamics of charge-transfer (CT) excitons at polymer/ZnO interface. The interfacial atomic structure, exciton density of states (DOS) and conversions between exciton species are examined from first-principles. The interfacial atomic structure and exciton DOS provide the basis to understand the interfacial charge separation. The conversions among the intermolecular, intramolecular, and CT excitons are examined in detail. The exciton dynamics exhibits both adiabatic and non-adiabatic characters. While the adiabatic transitions are facilitated by C=C vibrations along the polymer (P3HT) backbone, the non-adiabatic transitions are realized by exciton hopping between the excited states. We find that the localized ZnO surface states lead to localized low-energy CT states and poor charge separation. In contrast, the surface states of crystalline C60 are indistinguishable from the bulk states, resulting in delocalized CT states and efficient charge separation in polymer/fullerene (P3HT/PCBM) heterojunctions. The hot CT states are found to cool down in an ultrafast time scale and may not play a major role in charge separation of P3HT/ZnO. Finally we suggest that the dimensions of nanostructured acceptors can be tuned to obtain both efficient charge separation and high open circuit voltages.

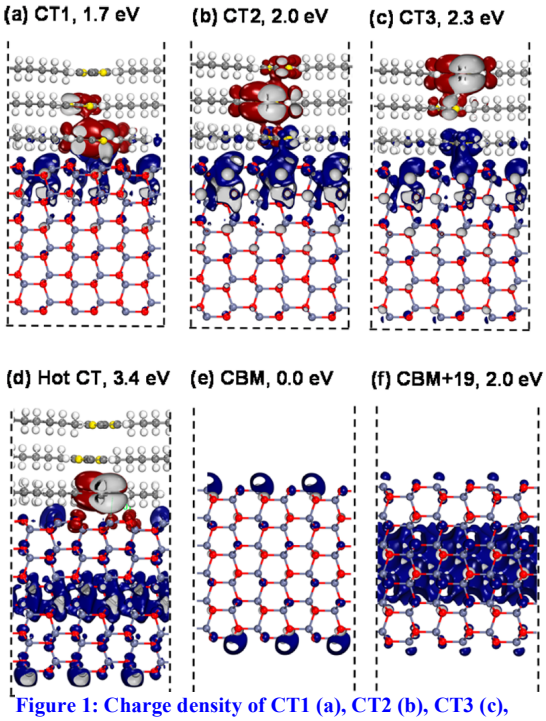
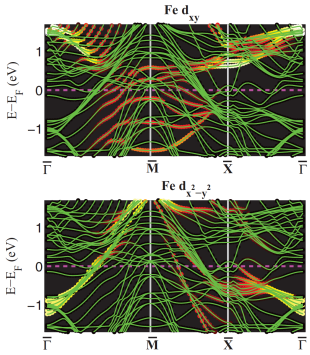


Figure 1: Charge density of CT1 (a), CT2 (b), CT3 (c), and the hot CT state with the hole on P1 (d). The red and blue color represents the charge density of the hole and the electron, respectively.

2. **Electric Field Control and Effect of Pd Capping on Magnetocrystalline Anisotropy in Fe-Pd Thin Films: A First-Principles Study** (Ong, et al., Phys. Rev. B 89, 094422, 2014)

Using *ab initio* electronic structure calculations, we have investigated the effect of electric field and of heavy metal cap of Pd on the magnetocrystalline anisotropy (MCA) of Fe-Pd ultrathin film. Analysis of the energy- and k-resolved distribution of the orbital-character of the minority spin band reveals that the perpendicular MCA of the uncapped film mainly arises from the spin-orbit coupling (SOC) between unoccupied Fe d_{xy} and occupied Fe dx_2-y_2 states. On the other hand, the SOC between the Pd- and Fe-derived *d*-states yields negative contributions to the MCA. We find that the sensitivity of the surface anisotropy energy to the applied electric field is 18 fJ/(Vm) and is due to changes in the occupation of the



surface Fe atoms dx_2-y_2 and (d_{xz}; d_{yz}) orbitals. We demonstrate that the thickness of the Pd cap has a dramatic effect on the MCA and can even switch the magnetization from out-of to in-plane orientation. The underlying origin is the change of the position and orbital character of the spin-polarized quantum well states induced in the Pd cap by varying its thickness. These results have important implications on exploiting heavy metals with large spin-orbit coupling (Ru, Pd, Ta, Pt, or Au) as contacts with ferromagnetic thin films to tailor the magnetic switching of spintronic devices by tuning the cap thickness.

Figure 2: Energy- and k-resolved distribution of the orbital character of the minority-spin band of the 9 ML FePd film.